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Preface

Fractal geometry applied to soil and related hierarchical systems

Complexity is an intrinsic quality of soil and related hierarchical Earth materials such as saprolite, rock, and marine sediments. It is the product of manifold feedbacks and multiscale interactions, which generate spatial and temporal heterogeneities in the properties and dynamics of natural porous media. Such heterogeneities can create substantial difficulties in environmental research since no experimental sample, site, or procedure is sufficient to fully represent the biogeochemical complexity that is present in the natural medium under study.

Because geometric measurements are at the heart of any research, the correct and efficient characterization of complex systems presents both a challenge and a necessity. Any measurement is based on some underlying model representation of the system in question. Fractal geometry has long been advocated as a better representation of complex particulate media as compared with simple Euclidean models based on straight lines and circle arcs. Recent developments in this field, including the application of information theory and multifractals to characterize natural hierarchical systems, were explored at the 6th International Workshop on "Fractal Mathematics Applied to Soil and Related Heterogeneous Systems" (PEDOFRACT 2004), which took place on July 2-6, 2004, at El Barco de Avila, Spain. This workshop attracted researchers from twelve countries and was supported by E.T.S.I. Agrónomos and Dpto. de Matemática Aplicada a la Ingeniería Agronómica, Universidad Politécnica de Madrid, Madrid, Spain. This special issue of Geoderma contains a collection of selected papers from PEDOFRACT 2004, plus some invited contributions.

Impressed and influenced by the informal style of the workshop, the co-editors of this special issue felt that the introduction should reflect the seminar discussions rather than contain a monotonous list of extended abstracts. As a result we have chosen to structure this foreword based on several key concepts that arose during the group discussions, and that were later expanded

upon via e-mail correspondence between participants. The ordering of these concepts is somewhat arbitrary, and does not reflect any implied ranking of importance.

1. Measurement and scale

Some degree of uncertainty is unavoidable in many fractal geometry applications since the measure is defined by counting instead of actually measuring. Counting and measuring are not the same. Errors associated with counting propagate through a hierarchy in currently unknown ways.

Although fractals should not be considered an ultimate model of scaling in the soil system, they do provide a balance between accuracy and clarity that may aid us in gaining insight into the sources and dynamics of complexity. Fractal geometry seemingly contradicts several commonly-held scientific viewpoints. As a result, it challenges us to examine these ideas more closely.

One example is the concept of "natural scales" as contrasted to "measurement scales." Fractal geometry uses the latter, and the limits of applicability of fractal scaling indicate changes in behavior that can be interpreted as the quantitative definition of natural scales. Fractal scaling laws may work at fine scales within relatively homogeneous sediments or at coarse scales with effective averaging that encompasses many relatively homogeneous parts. Breaks in fractal scaling may reflect intermediate scales where heterogeneities are not numerous enough to be ensemble-averaged. Another example is the concept of parameter estimation. If soil properties and/or behavior are simulated as emerging systems using fractal models, the ubiquitous concept of inverse solutions to estimate model parameters loses its value.

2. Homogeneity and heterogeneity

Geometrical multifractals and entropy-based measures challenge our traditional conceptions about soil

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variability. Such analyses suggest that the most heterogeneous systems are made up of relatively homogenously-weighted component parts. In soil physics, for example, soils classified as sands are usually considered to be homogenous, whereas clays are regarded as heterogeneous. According to the fractal viewpoint, however, sand is heterogeneous because it contains approximately equal masses of solid particles in all possible size classes, while clay is homogeneous because most of the solid particles are concentrated into a few small size classes. This reversal of definitions may represent the first glimmering of a future paradigm shift that could have important implications for our understanding of soil variability, and how it influences processes such as water flow and contaminant transport.

Fractal geometry is currently one of the best tools to address extreme events and rare occurrences. Rare occurrences at fine measurement scales tend to be the most important ones on coarse scales. For example, macropores are rare occurrences in traditional soil samples taken to measure hydraulic properties at the core scale. However, the hydrologic behavior of soil at the pedon scale is in many cases defined by macropores. Multifractals and distribution tail studies show much promise for characterizing and predicting these extreme phenomena.

3. Structure and function

Relationships between structure and function are revealed and studied in many disciplines, e.g. plant science, molecular biology, sociology, just to name a few. The hydrologic functioning of soils, for example, is defined by the structure of pathways and voids available for water storage and movement. In turn, pore space geometry is strongly influenced by the functioning of soils within the hydrologic cycle. This relationship has a multitude of feedbacks that modify function according to changes in structure, and vice versa.

Fractal geometry has provided a theoretical and practical framework for relating structure to function in natural porous media, and for understanding the associated feedbacks. The applied aspects of this relationship can be summarized as follows:

- proper simulation of soil/sediment structure to generate equiprobable random fields of soil hydraulic properties or equiprobable pore spaces to research soil functioning in water and contaminant transport, and microbial activity;
- probabilistic identification of breakthrough pathways in structure as a precondition to scale soil functional behavior to coarser scales.

The challenge now is to see whether fractal geometry can be helpful to quantify and simulate pore connectivity and reveal the hierarchy of transport pathways. The fact that randomly created structures become fractal at the percolation threshold lends support to the viability of linking static fractal structures to dynamics via connectivity.

4. Cognition and recognition

While the complexity of transport pathways in disordered systems may be easy to perceive, it is often difficult to represent in mathematical terms without making strong simplifying assumptions. This implies that several different model structures can be consistent with the available observations. This multiplicity of possible models reflects the multiplicity of conceptual approaches available for representing complex subsurface processes in mathematical forms that are tractable within the limitations of existing computer and measurement technologies.

Applications of fractal geometry remain dependent on human cognition and often contain a subjective component. Separation of pores and solids (thresholding) prior to analyzing digitized images of soil thin sections for their fractal properties, and the manual identification of scaling limits are common examples. Subjective decisions about scaling limits should be abandoned in favor of objective statistical approaches that do not require contemplation of the underlying perceptions responsible for a particular choice.

As we move away from subjective decisions in analysis it is interesting to apply our analytical tools to manmade hierarchical structures. For example, what does the apparent fractal scaling of soil taxonomic systems and other classification schemes, tell us about human cognition? Are the fractal structures a product of decisions made by the scientists who devised the system, or a result of the choices made by those that analyzed them?

5. Data and analysis

In many applications of fractal geometry, there appears to be a growing trend towards increasingly complex analyses being performed on simpler and simpler data sets. For example, it is possible to analyze basic soil textural class data using a variety of multifractal, iterated function system (IFS), and entropy-based techniques. The outcomes of this trend are uncertain. Sophisticated analyses of simple data sets can yield predictions about behavior at finer and/or coarser scales.

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Ultimately, however, more detailed data sets are needed for testing model predictions.

Advanced measurement technologies, such as laser diffractometry, scanning electron microscopy, computer assisted tomography, and remote sensing, often provide large volumes of data. Such data sets provide new opportunities for determining the information content and complexity of natural systems. However, there is a clear need for protocols to collapse these data into meaningful and management-sensitive parameters.

Fractal geometry has been instrumental in developing measures of the irregularity observed in lines, surfaces, and volumes. There is no doubt that some of these measures are extremely useful for discriminating between natural systems. Assuming the underlying geometry of soils and/or rocks is fractal may permit the efficient parameterization of spatially- and temporally-dense data sets. In particular, more experience is needed with the use of fractal and multifractal analyses in "image texture" characterization. We need to identify which of the myriad of parameters available relate best to function, and/or are most useful for compressing high volume data sets.

6. Uses and abuses

Pseudo-fractal scaling can be found in systems that have been generated without any scale-invariant repetitive process. Therefore, hierarchical scaling is the necessary condition to apply fractal geometry. However, the sufficient condition is the identification of physical, chemical or biological processes that are able to produce fractal scaling. Fragmentation is one example, but more need to be discovered.

Monofractal models are often fitted to data sets by linear regression following log-transformation of the relevant variables. It is well known that such analyses bias some data towards being more "relevant" than others, which is not be a desired effect. Since only small differences in estimates of the fractal dimension for a system can have profound effects on a multitude of biogeochemical properties and processes, the investiga-

tion of alternative parameter estimation methods such as non-linear regression and maximum likelihood deserves more attention. At the very least, researchers need to routinely check the residuals from linear regression analyses for normality, autocorrelation, and homoscedasticity. Without attention to these details, the widespread use of off-the-shelf computer programs for data analysis can easily lead to misapplication of statistical techniques and erroneous conclusions about the applicability of fractal models.

Readers of this special issue of Geoderma should be able to detect manifestations of some of the concepts and tensions discussed above in individual papers, or within certain thematic groupings. Taken as a whole, the research presented here provides a representative sample of the ongoing international effort to expand the use of fractal models in the Earth sciences. The interactions and discussions stimulated by this workshop suggest that there are many more avenues for research that can be pursued in this context. With this introductory note we hope to broaden these discussions by involving the journal readership.

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